2-Butanol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -70.5 °C

Global applicability domain: Inside

Local applicability domain index: 8.13e-01

Confidence level: 3.96e-01

Nearest Neighbors from the Training Set

Image not found
2-Butanol
Measured: -115
Predicted: -70.5

Image not found
2,2-Dimethylpropanol
Measured: 52.5
Predicted: -31.2

Image not found
Isopentyl alcohol
Measured: -117
Predicted: -96.2

Image not found
2-Methyl-1-propanol
Measured: -108
Predicted: -103

Image not found
tert-Butyl alcohol
Measured: 25.4
Predicted: -11.0